Supplementary materials

Synthesis, DNA binding and molecular docking studies of Dimethylaminobenzaldehyde based bioactive Schiff bases

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Figure Captions

Figure S17: Mass spectrum of compound **1**.

Figure S18: Mass spectrum of compound **2**.

Figure S19: Mass spectrum of compound **3**.

Figure S20: Mass spectrum of compound **4**.

Figure S21: Mass spectrum of compound **5**.

Figure S22: Mass spectrum of compound **6**.

Figure S23: Mass spectrum of compound **7**.

Figure S24: Mass spectrum of compound **8**.

Table Captions

Table S1. Pharmacokinetic parameters important for good oral bioavailability of heterocyclic Schiff base derivatives (**1-8**)

Molecular Docking Study

Autodock 4.1 software was used to study the molecular docking. It is an interactive molecular graphics programme to study the docking modes of protein, different types of enzymes and DNA. ChemSketch (http://www.acdlabs.com) was used to draw the structure of compounds, smiles of compounds were collected from mole inspiration (http://www.molinspiration.com/) and ligand in PDB format was obtained from smile converter software (https://cactus.nci.nih.gov/translate/). From the protein data bank (http://www.rcsb.org./pdb), the

crystal structure of B-DNA dodecamer d(CGCGAATTCGCG)$_2$ (PDB ID: 1BNA) was downloaded. PyMol (http://pymol.sourceforget.net/) molecular graphics program was used to visualize the docked pictures.

In vitro Antibacterial Susceptibility Assay

The *Escherichia coli*, *Klebsiella pneumoniae*, *Pseudomonas aeruginosa* and S*taphylococcus aureus* strains were tested according to standard NCCLS protocol as per our previous work. The experiment was performed in triplicate under strict aseptic conditions. The antibacterial activity for the synthesized Schiff bases (**1-8**) was expressed in terms of the average of the diameter of zone of inhibition (in mm) produced by the respective compound.

Pharmacological Investigation

The molecular properties and Lipinski rule of five for the synthesized compounds were determined by online software Mol inspiration Chemo Informatics. According to the Lipinski "Rule of Five", the synthesized compounds have good membrane permeability, log P $\leq$ 5, molecular weight $\leq$ 500. The Calculated pharmacophore or drug-like properties of the compounds (**1-8**) shows that all the compounds does not violate from Lipinski rule and all the properties are in considerable range shown in **Table S1.**

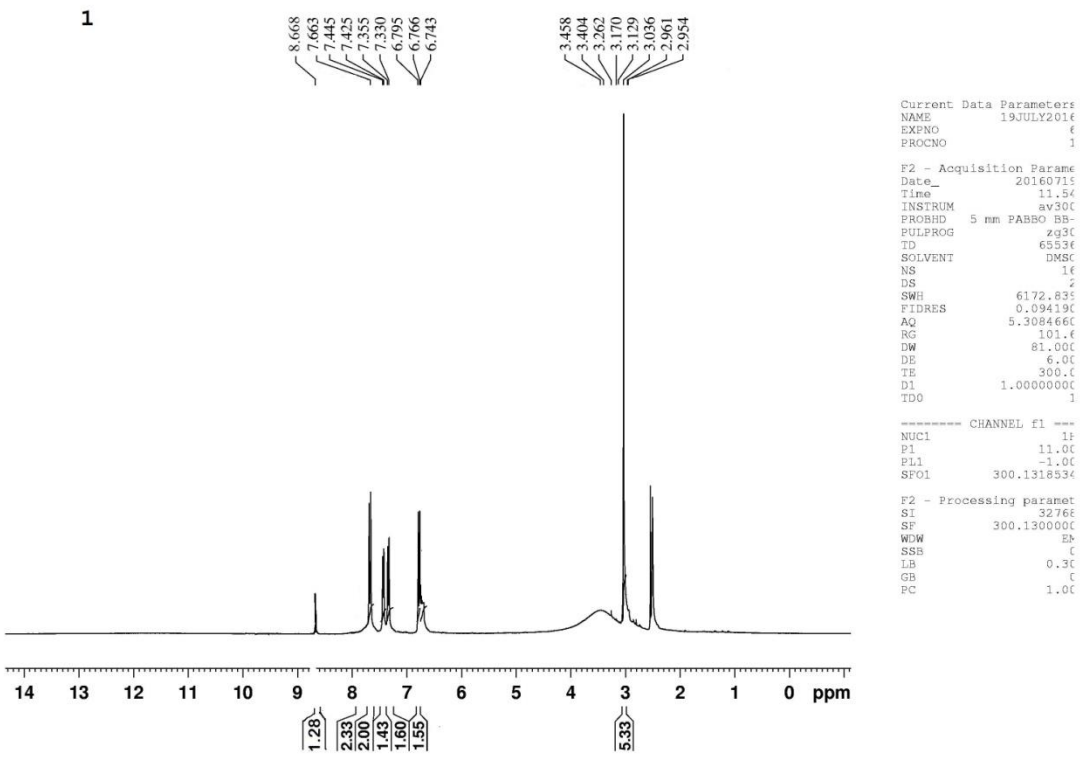

Figure S1: ^{1}H NMR spectrum of compound **1**.

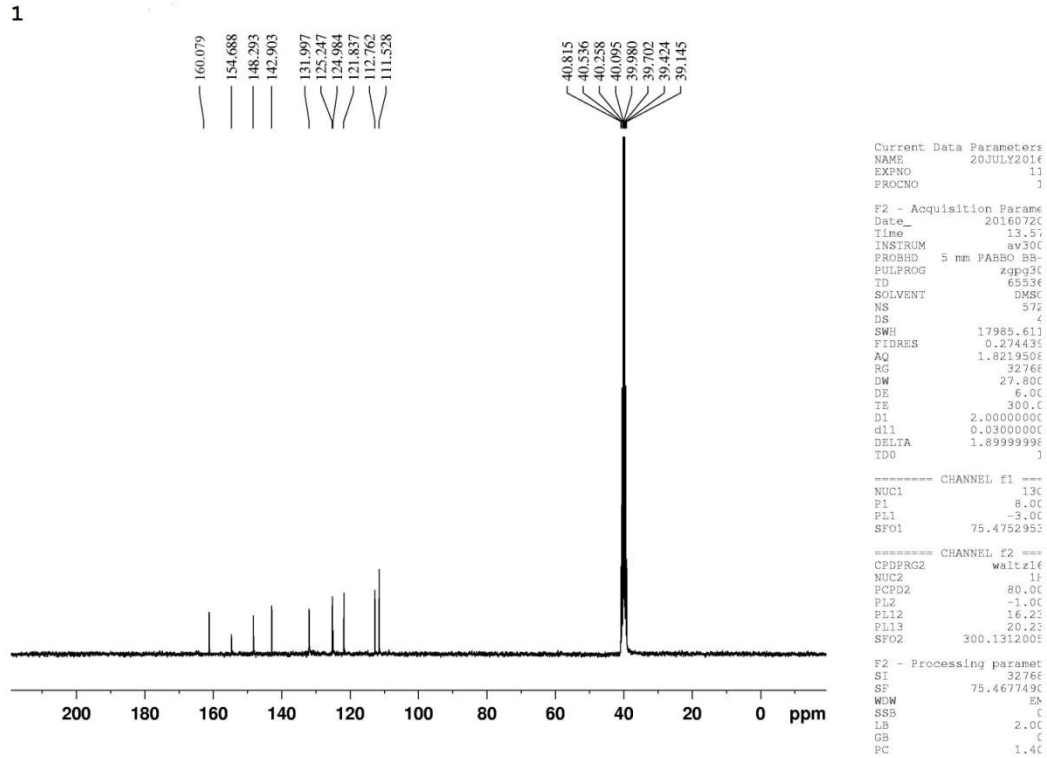

Figure S2: ^{13}C NMR spectrum of compound **1**.

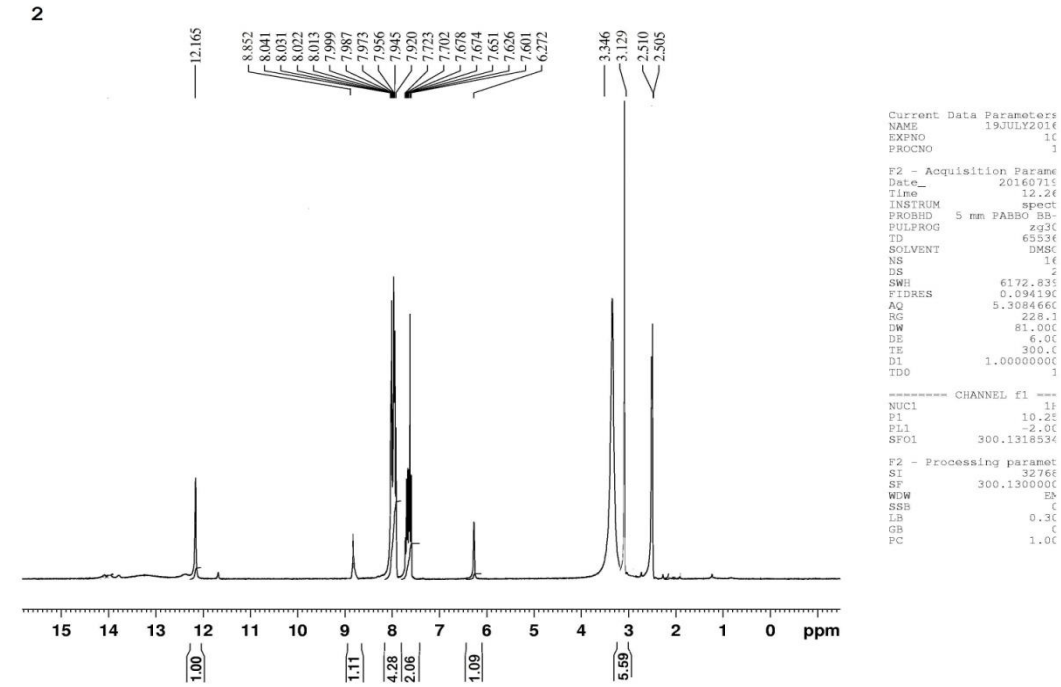

Figure S3: ^{1}H NMR spectrum of compound **2**.

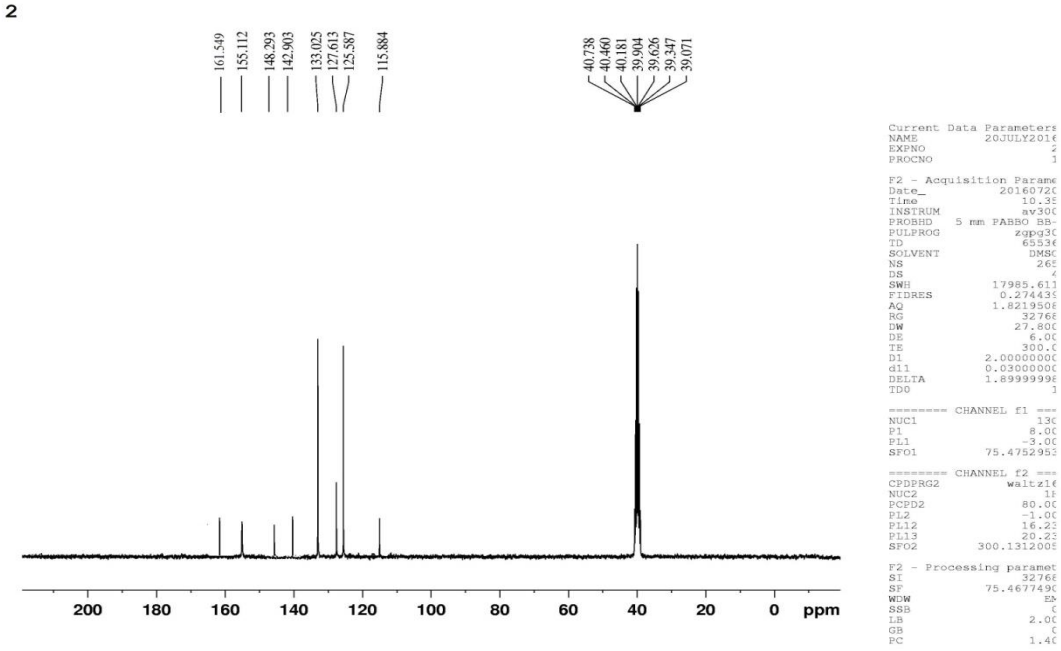

Figure S4: ^{13}C NMR spectrum of compound **2**.

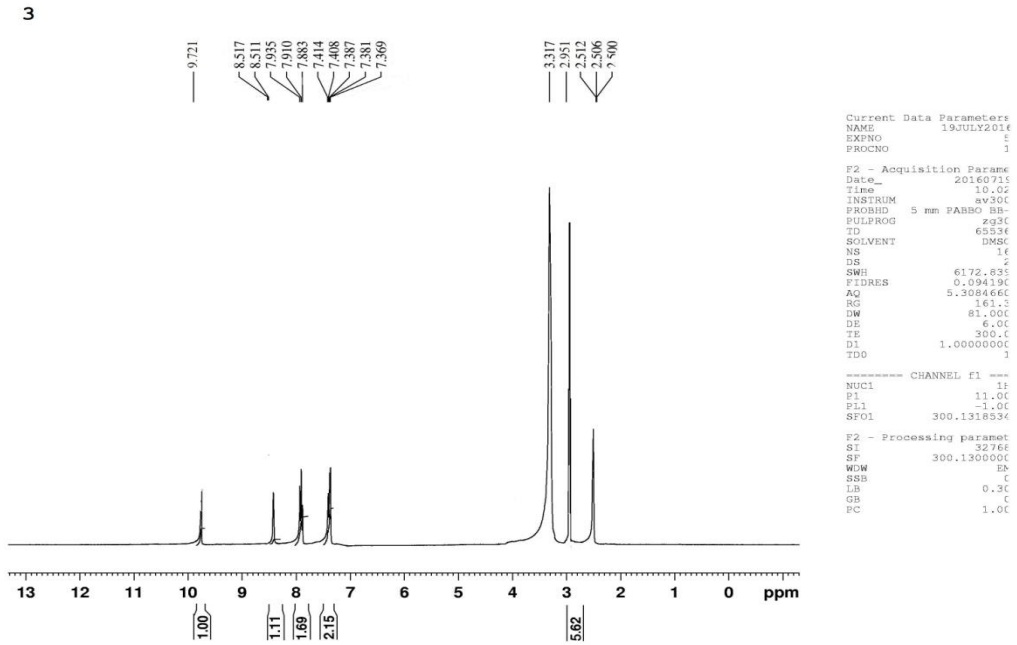

Figure S5: ^{1}H NMR spectrum of compound**3**.

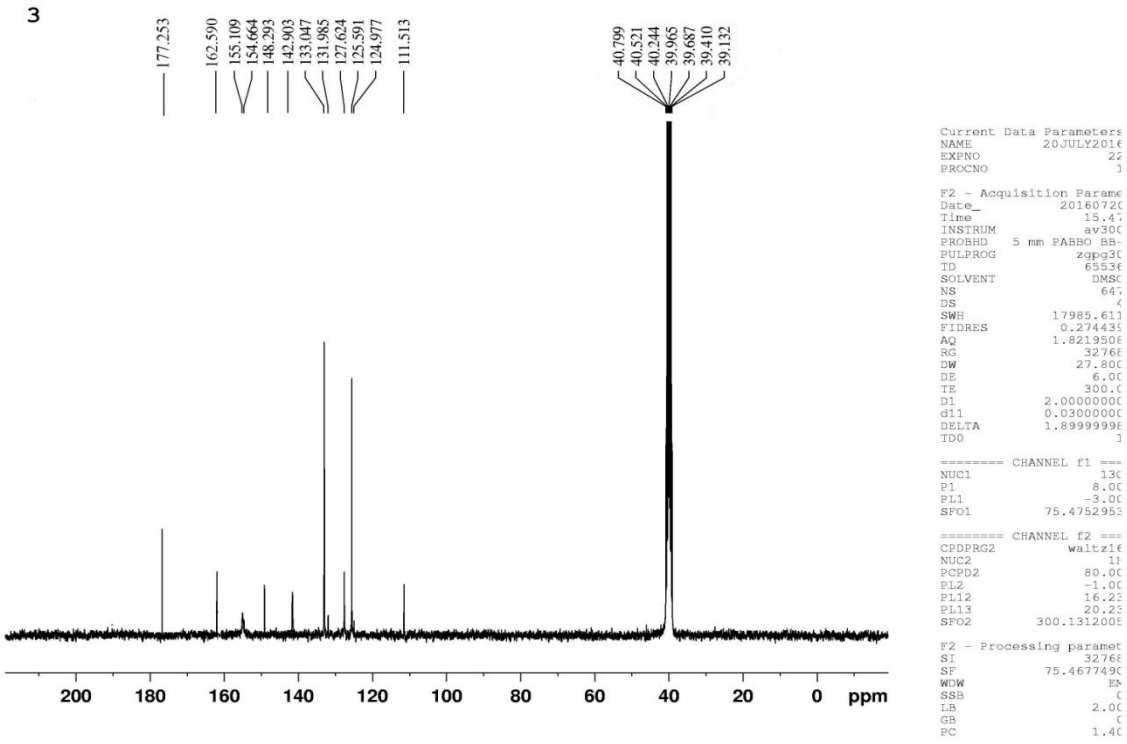

Figure S6: ^{13}C NMR spectrum of compound **3**.

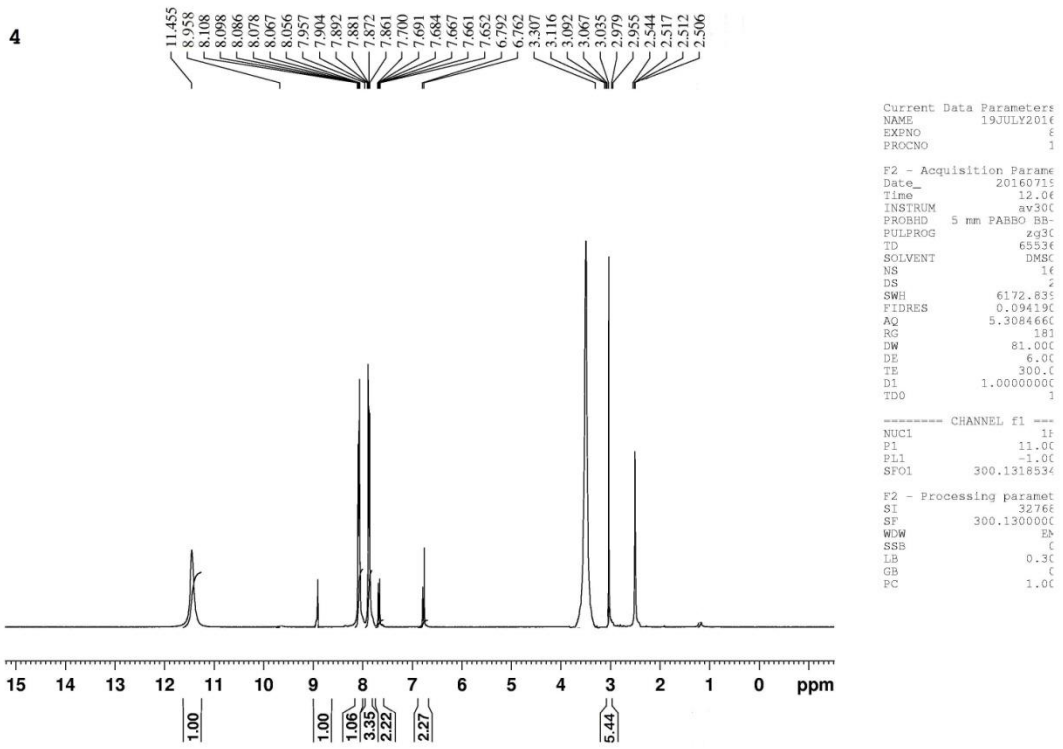

Figure S7: ^{1}H NMR spectrum of compound **4**.

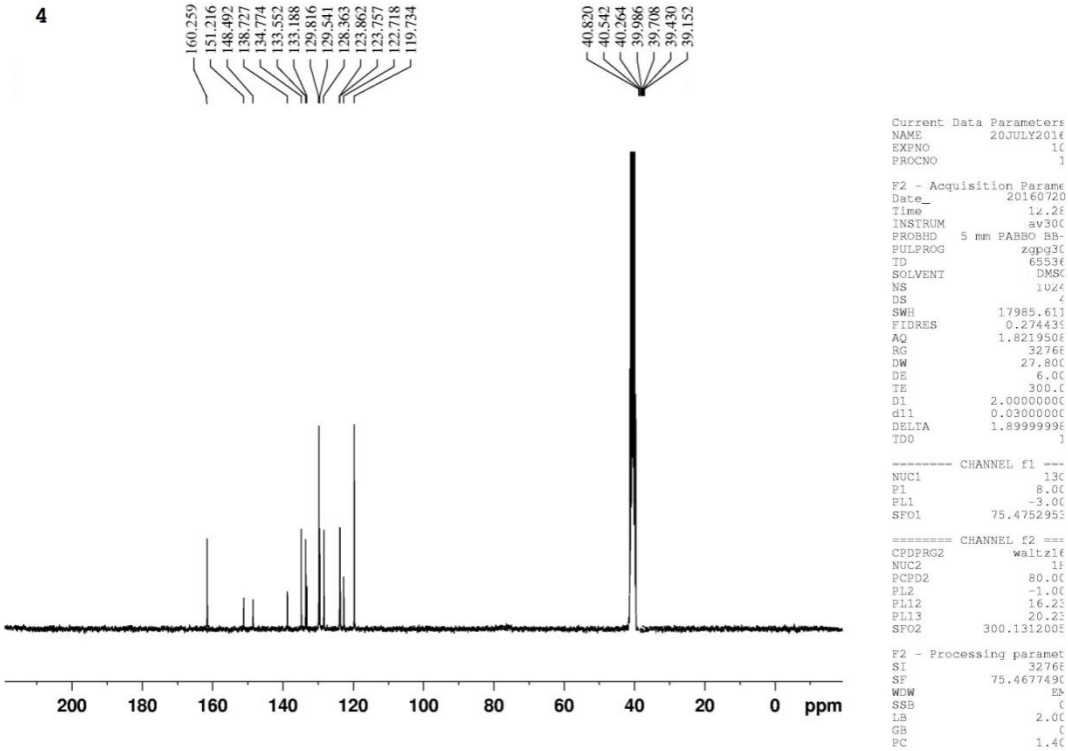

Figure S8: ^{13}C NMR spectrum of compound **4**.

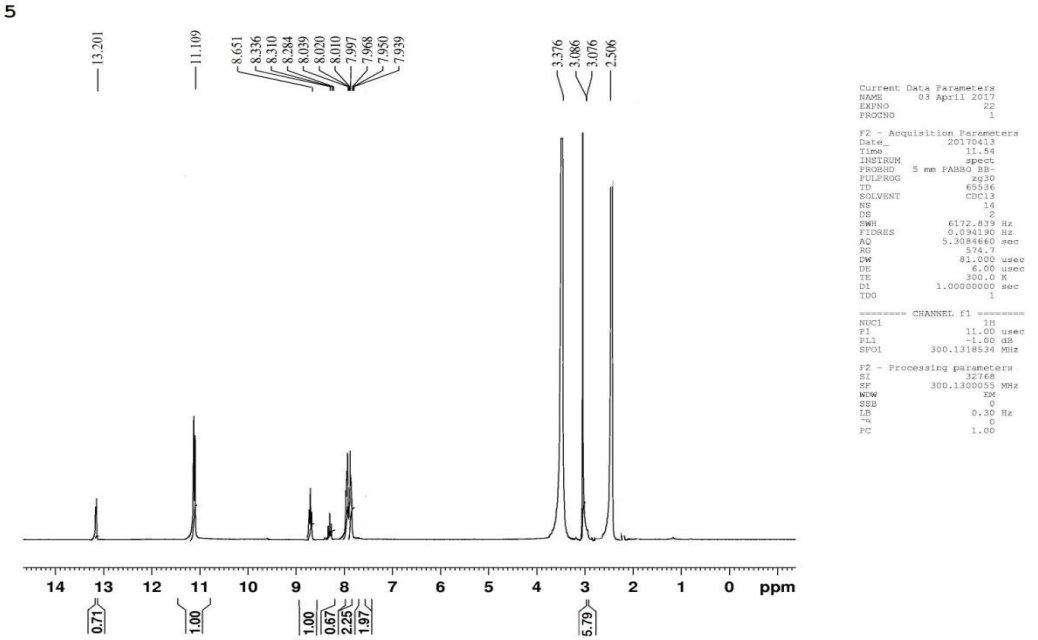

Figure S9: ^{1}H NMR spectrum of compound **5**.

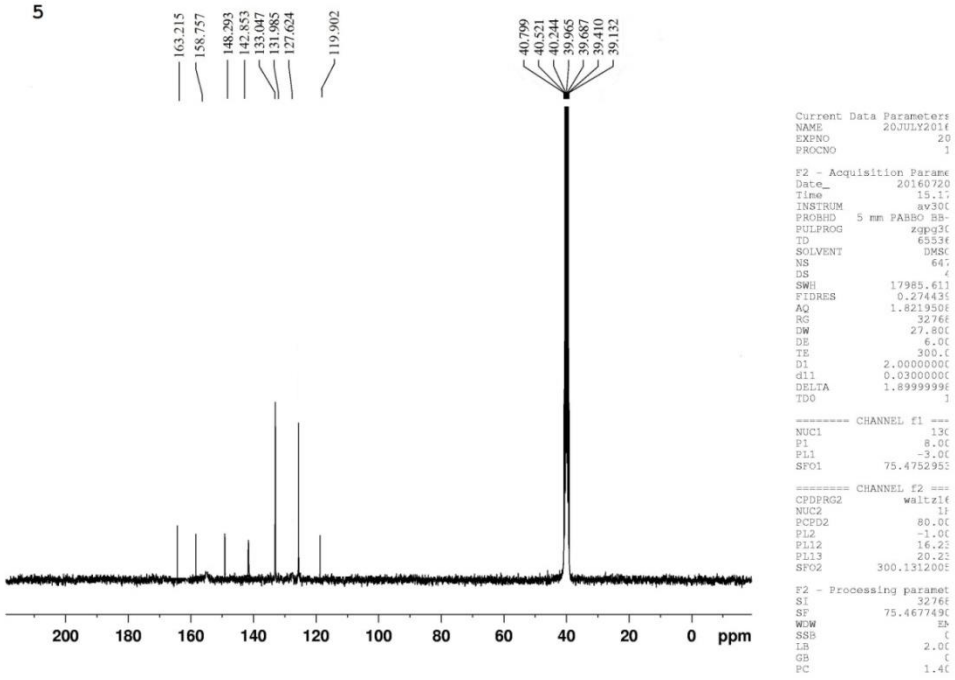

Figure S10: ^{13}C NMR spectrum of compound **5**.

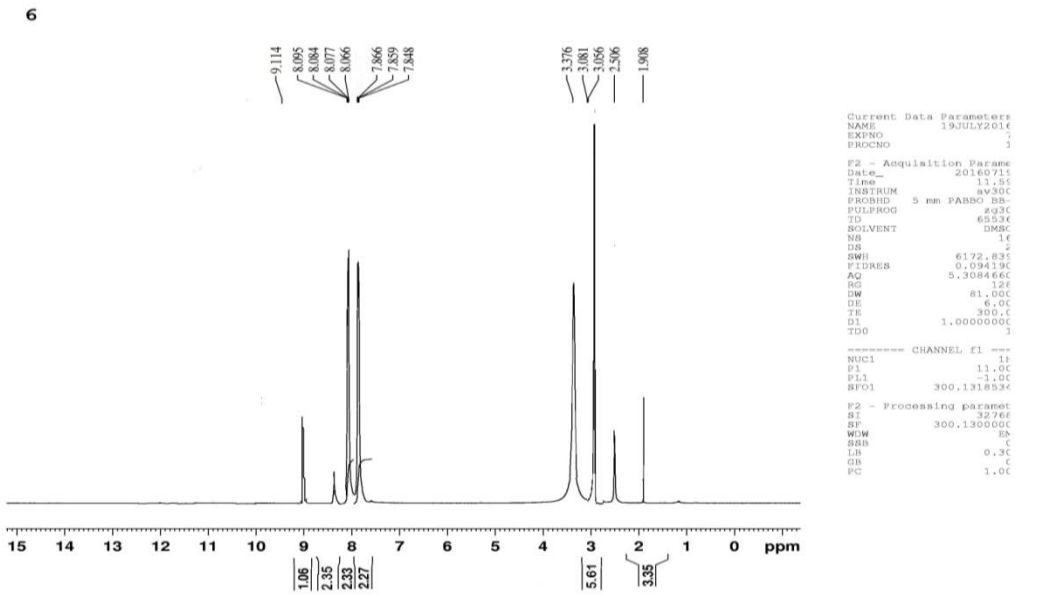

Figure S11: ^{1}H NMR spectrum of compound **6**.

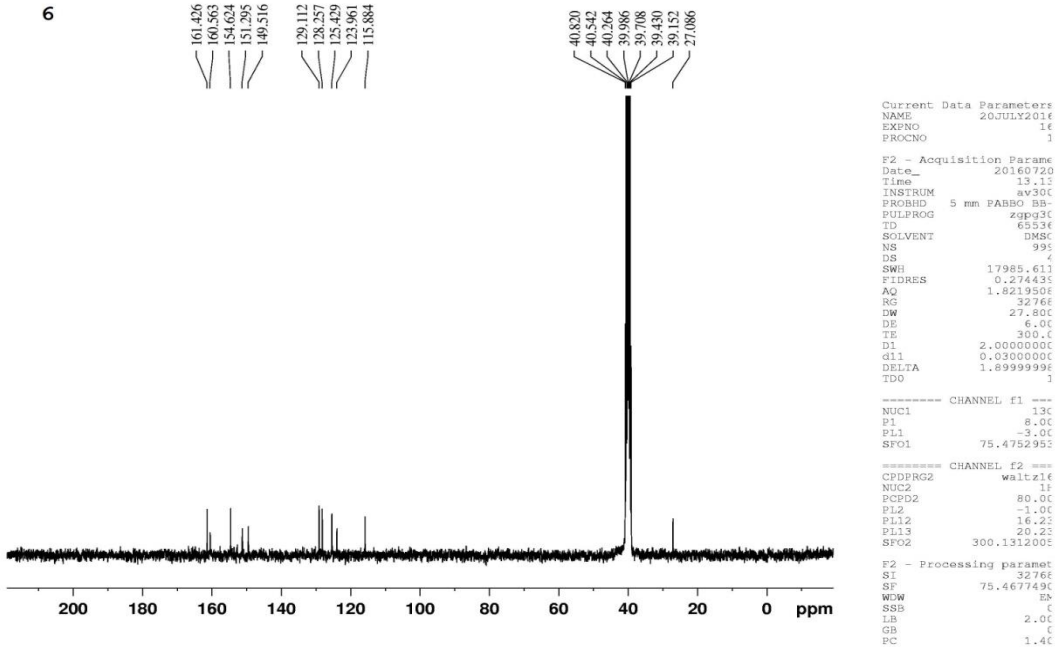

Figure S12: ^{13}C NMR spectrum of compound **6**.

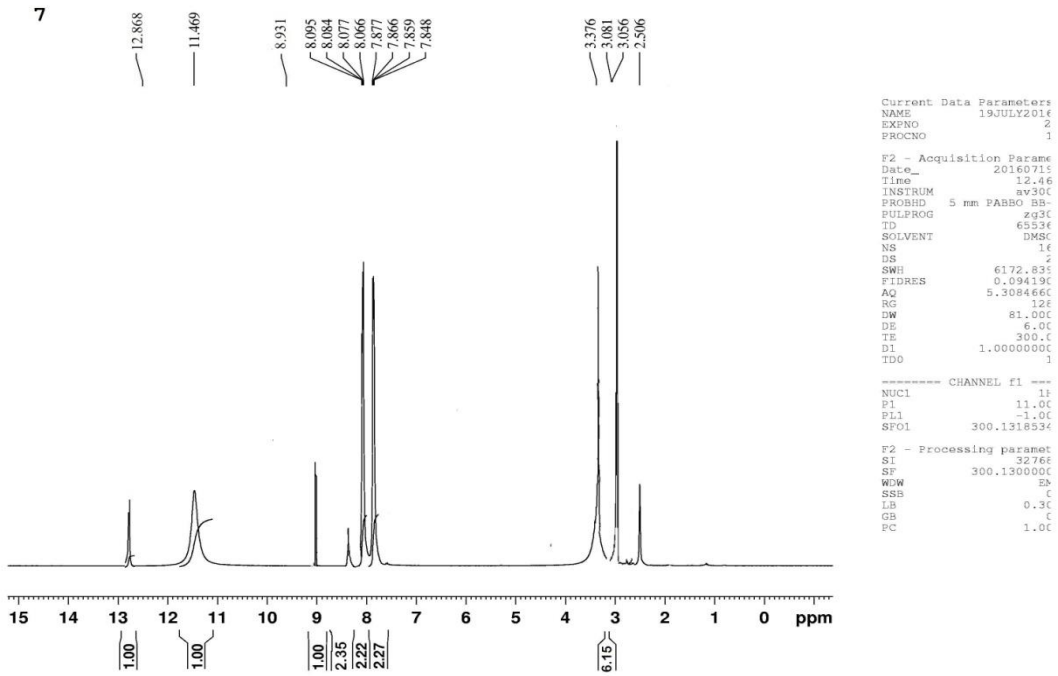

Figure S13: ^{1}H NMR spectrum of compound **7**.

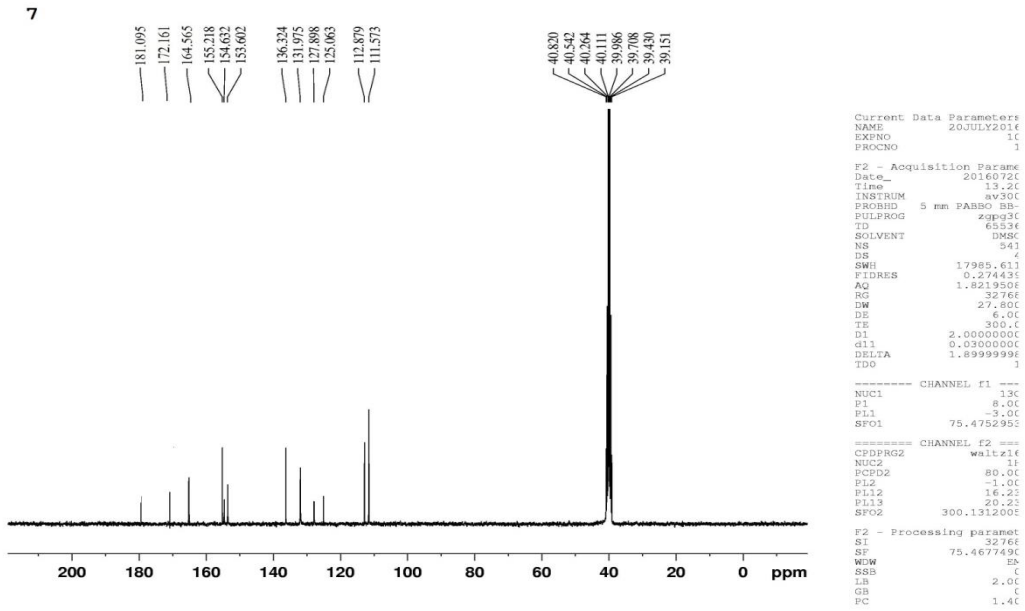

Figure S14: ^{13}C NMR spectrum of compound **7**.

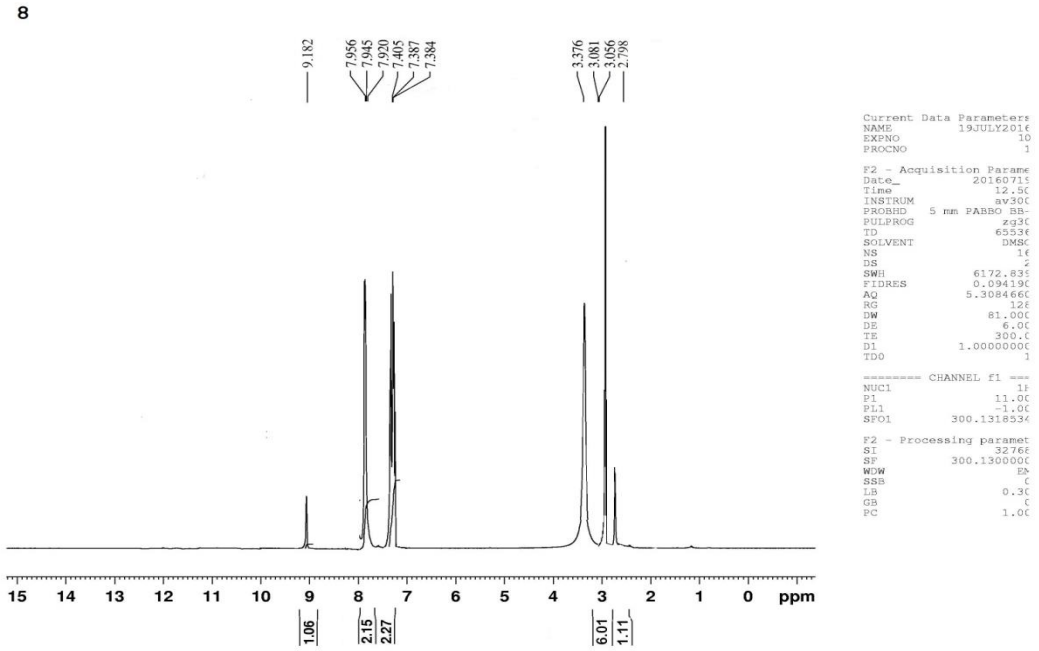

Figure S15: ^{1}H NMR spectrum of compound **8**.

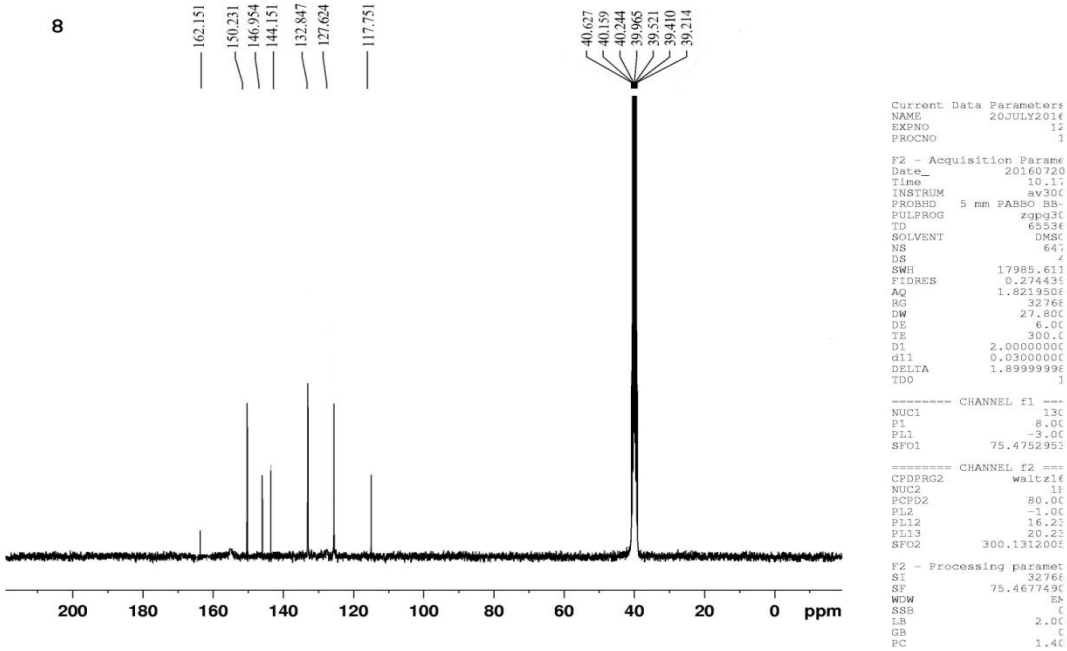

Figure S16: ^{13}C NMR spectrum of compound 8.

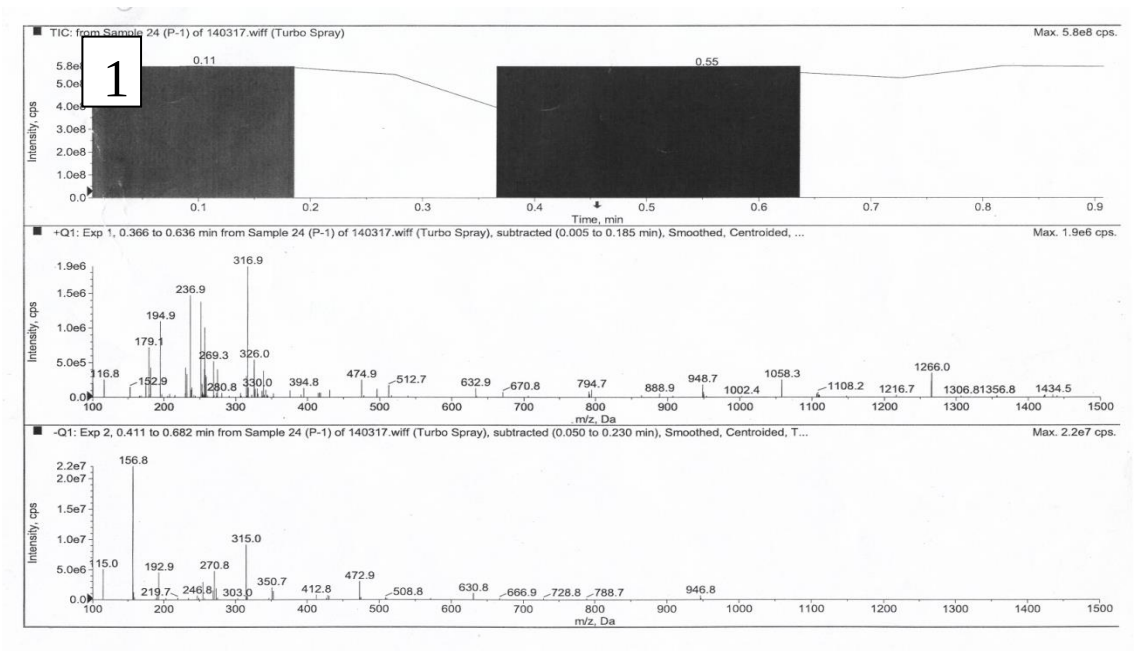

Figure S17: Mass spectrum of compound **1**.

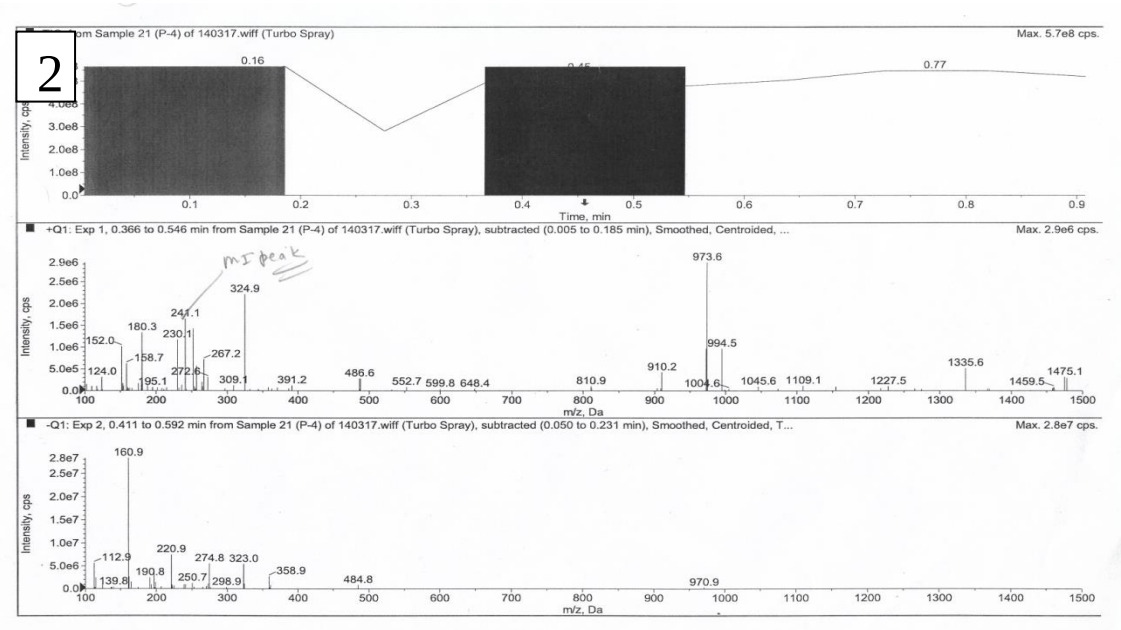

Figure S18: Mass spectrum of compound **2**.

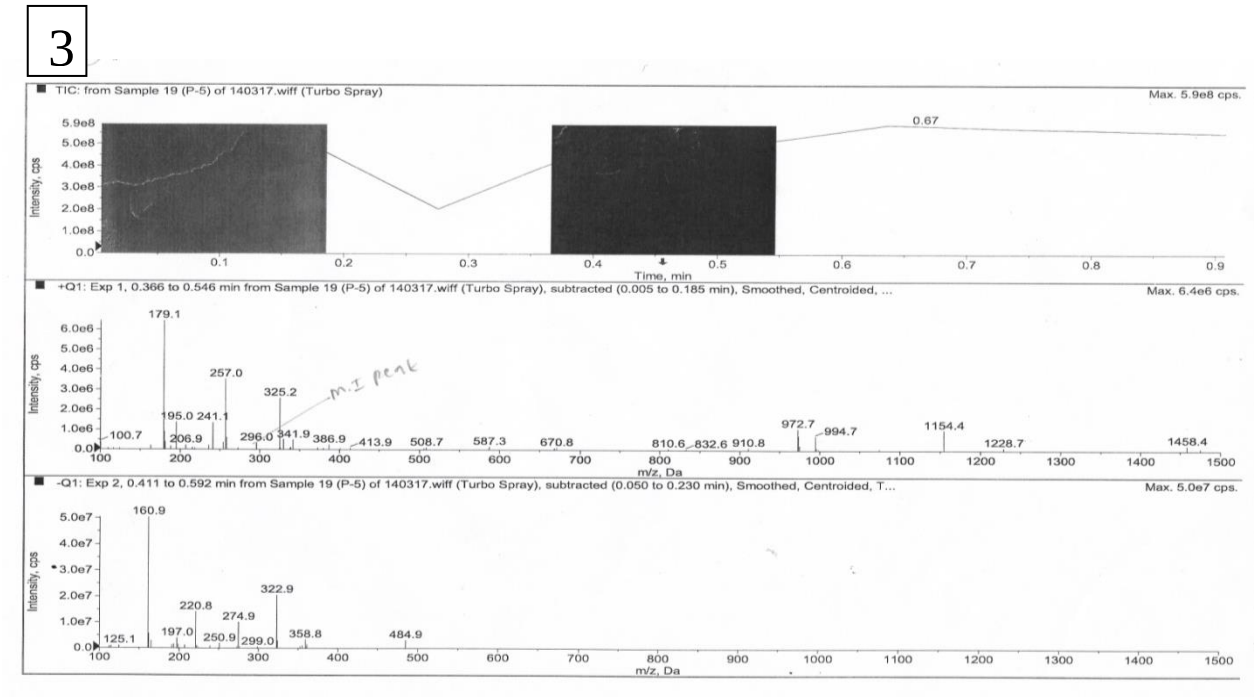

Figure S19: Mass spectrum of compound **3**.

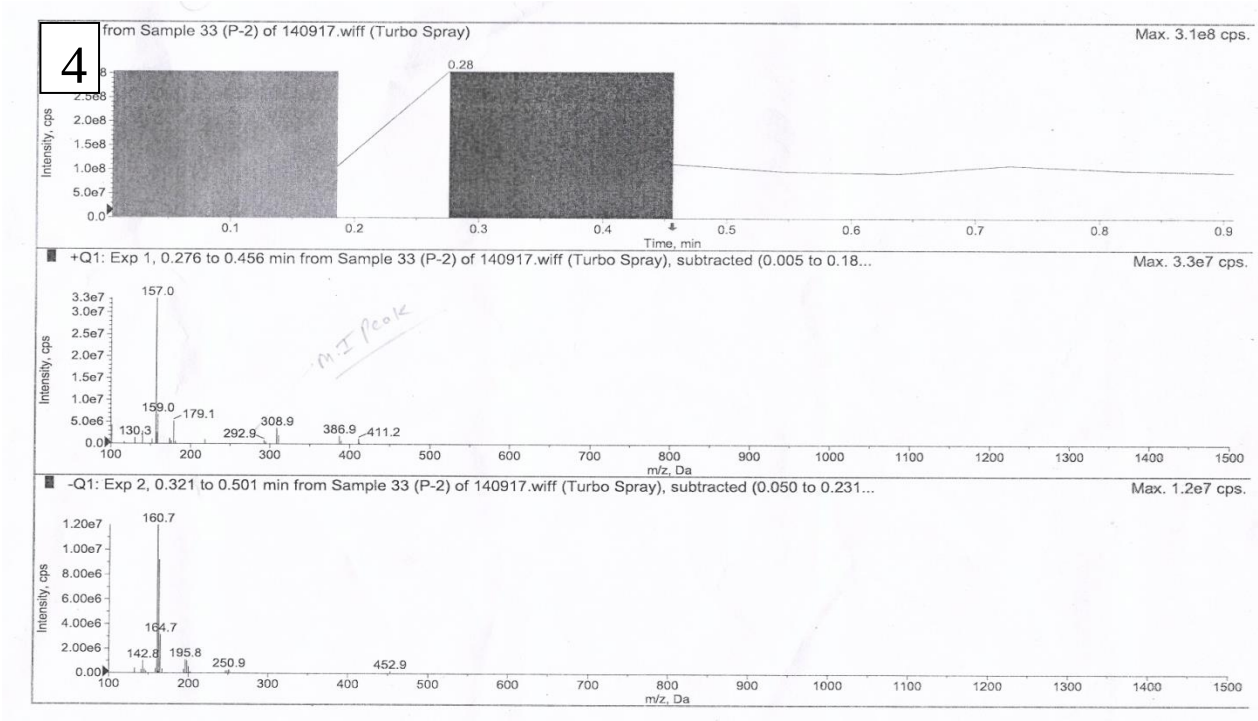

Figure S20: Mass spectrum of compound **4**.

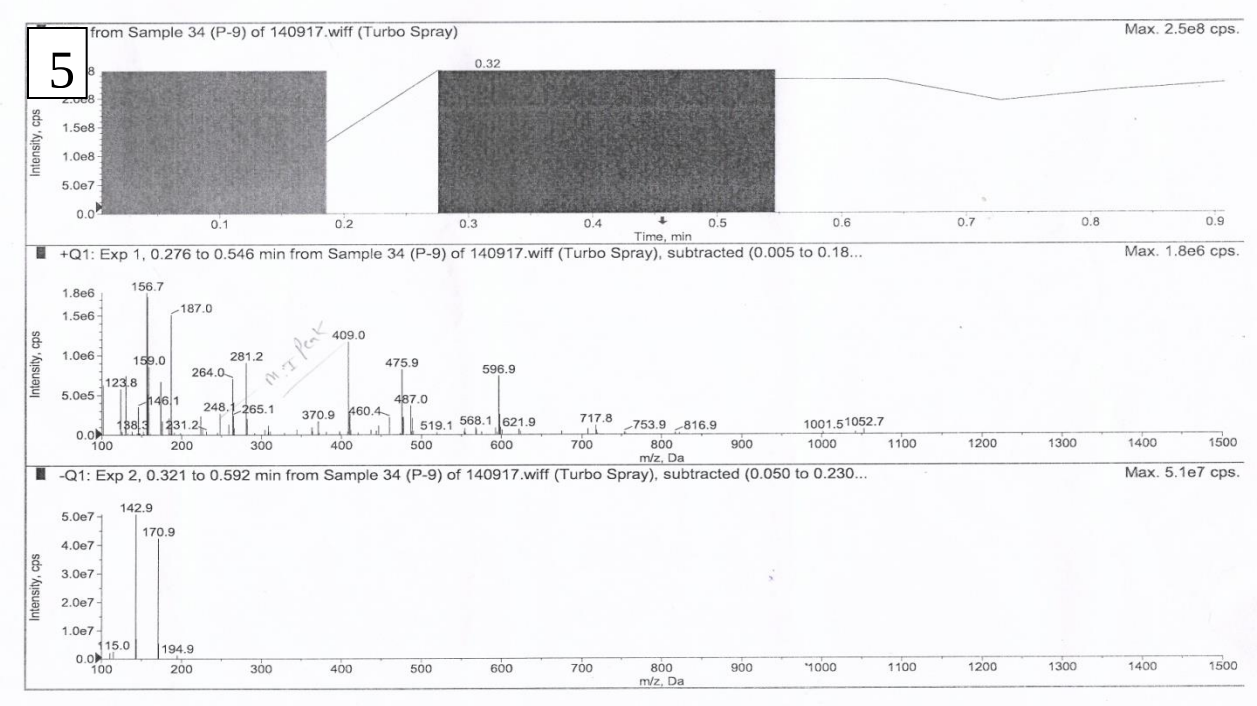

Figure S21: Mass spectrum of compound **5**.

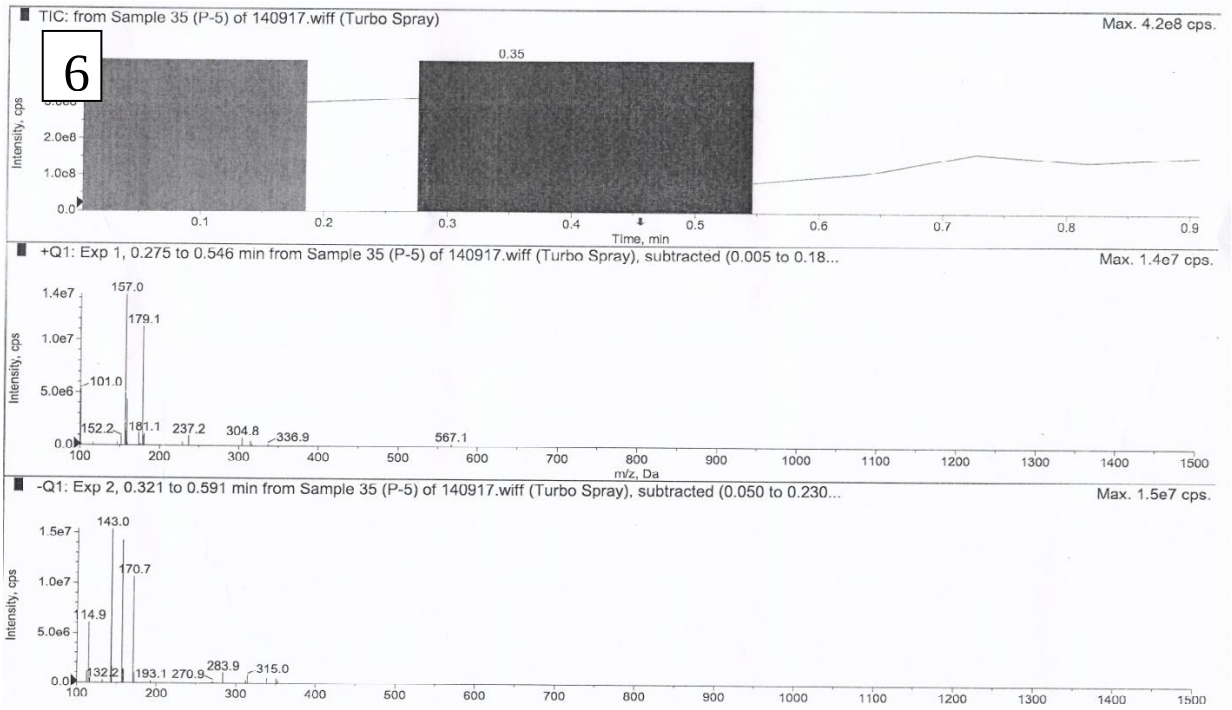

Figure S22: Mass spectrum of compound **6**.

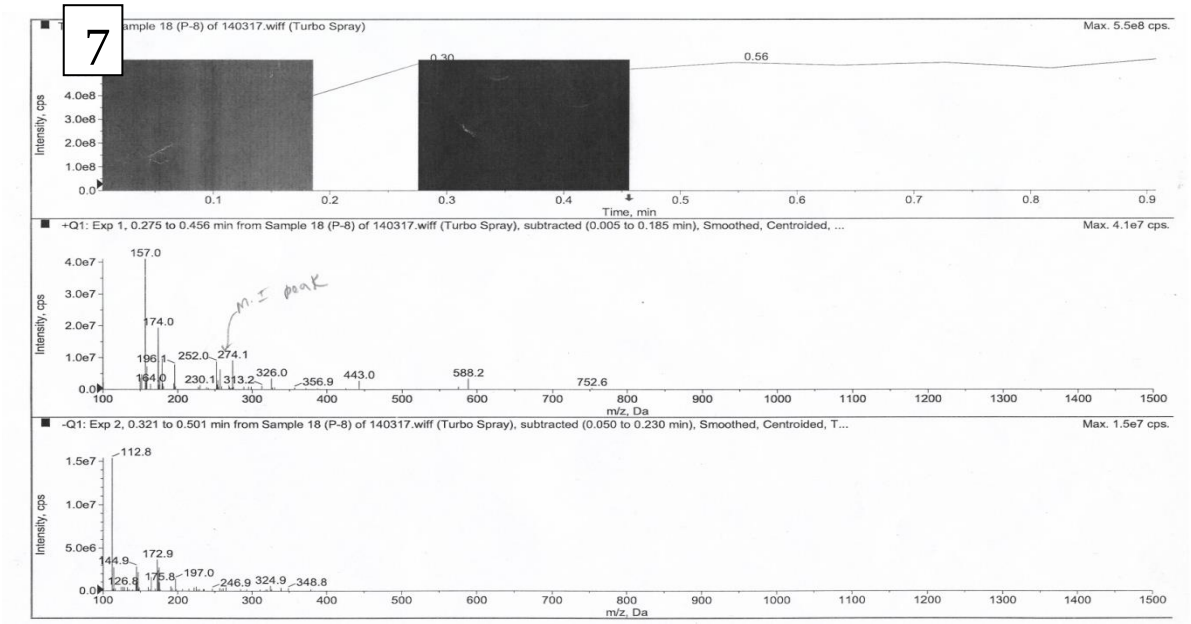

Figure S23: Mass spectrum of compound **7**.

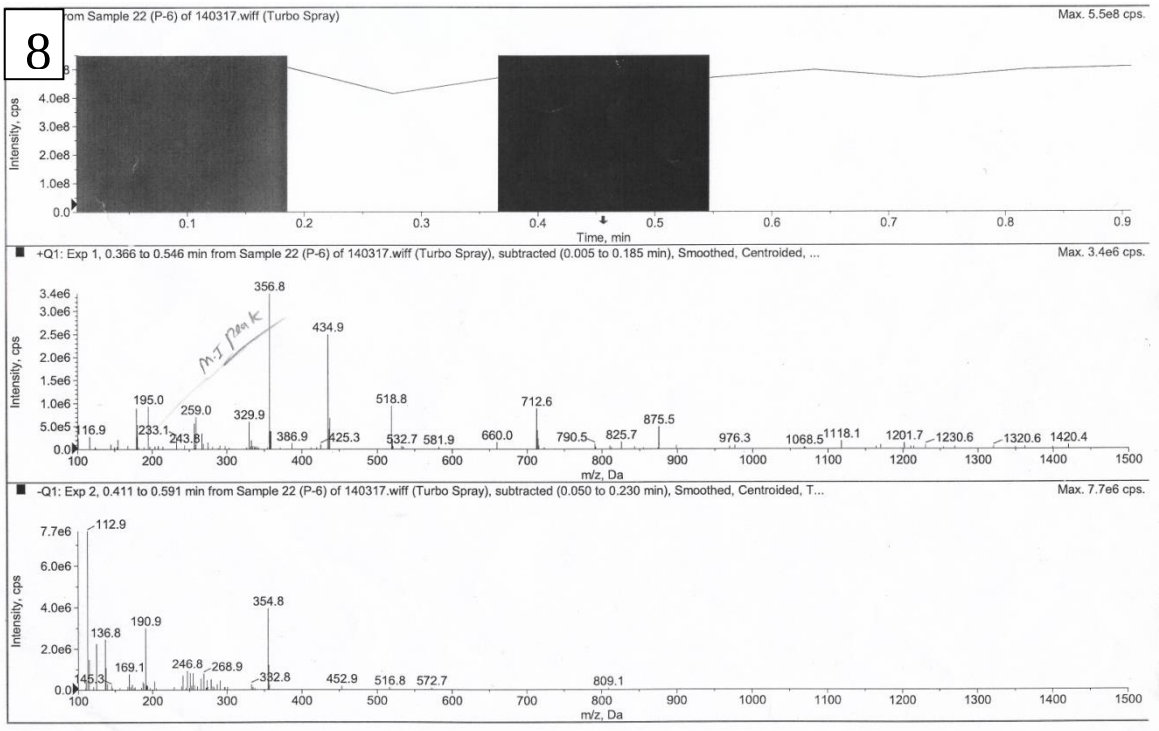

Figure S24: Mass spectrum of compound 8.

Table S1. Pharmacokinetic parameters important for good oral bioavailability of heterocyclic Schiff base derivatives (**1-8**)

Compound	**% ABS**	**Volume (A3)**	**TPSA (A2)**	**NROTB**	**n-ON acceptor**	**n-OHNH donors**	**miLog *P***	**MW**	**Lipinski's violations**
1	82.84	244.82	73.69	4	6	0	2.62	318.40	0
2	91.45	229.36	47.21	3	4	1	2.53	344.4	0
3	98.67	244.82	42.57	3	4	0	3.79	420.5	0
4	91.45	273.68	49.33	3	4	1	3.58	370.5	0
5	97.87	219.69	58.64	3	5	1	2.12	446.6	0
6	98.04	238.74	29.17	3	3	0	3.11	509.0	0
7	86.93	242.86	62.84	3	5	0	2.67	514.0	0
8	93.72	208.67	42.68	3	4	0	2.34	509.0	0
Rule	-	-	-	-	<10	<5	≤5	< 700	≤1

% ABS, percentage of absorption; **TPSA**, topological polar surface area; **NROTB**, number of rotatable bonds; **n-ON**, number of hydrogen bond acceptors; **n-OHNH**, number of hydrogen bond donors; **miLogP**, logarithm of compound partition coefficient between n-octanol and water; **MW** = molecular weight.